Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1611bxv

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	DEC 23	New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/ USPAT2
NEWS	4	JAN 13	IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
NEWS	5	JAN 13	New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to INPADOC
NEWS	6	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS	7	JAN 17	IPC 8 in the WPI family of databases including WPIFV
NEWS	8	JAN 30	Saved answer limit increased
NEWS	9	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS	10	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS	11	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS	12	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS	13	FEB 28	MEDLINE/LMEDLINE reload improves functionality
NEWS	14	FEB 28	TOXCENTER reloaded with enhancements
NEWS	15	FEB 28	REGISTRY/ZREGISTRY enhanced with more experimental spectral property data
NEWS	16	MAR 01	INSPEC reloaded and enhanced
NEWS	17	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS	18	MAR 08	X.25 communication option no longer available after June 2006
NEWS	19	MAR 22	EMBASE is now updated on a daily basis
NEWS	20	APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS	21	APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS	22	APR 04	STN AnaVist $500 visualization usage credit offered
NEWS	23	APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS	24	APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS	25	APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected

NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT
http://download.cas.org/express/v8.0-Discover/

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* *

COMPLETE THE STN SURVEY - APRIL 27 THROUGH MAY 31

Dear valued STN customer,

In an effort to enhance your experience with STN, we would like to better understand what you find useful. Please take approximately 5 minutes to complete a web survey.

If you provide us with your name, login ID, and e-mail address, you will be entered in a drawing to win a free iPod(R). Your responses will be kept confidential and will help us make future improvements to STN.

Take survey: http://www.zoomerang.com/survey.zgi?p=WEB2259HNKWTUW

Thank you in advance for your participation.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:13:09 ON 05 MAY 2006

=> FILE CASREACS
'CASREACS' IS NOT A VALID FILE NAME
SESSION CONTINUES IN FILE 'HOME'
Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

=> FILE CASREAC

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'CASREACT' ENTERED AT 10:13:35 ON 05 MAY 2006
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE CONTENT:1840 - 30 Apr 2006 VOL 144 ISS 18

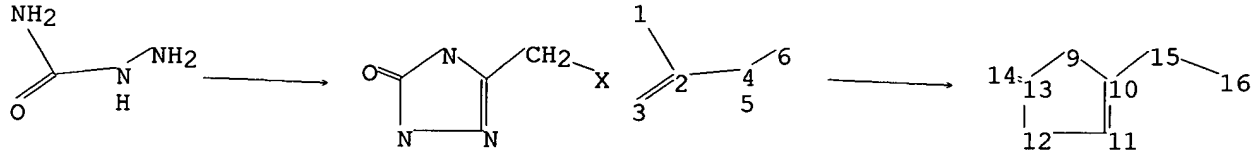
New CAS Information Use Policies, enter HELP USAGETERMS for details.

****
*
* CASREACT now has more than 10 million reactions
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\10524866.str

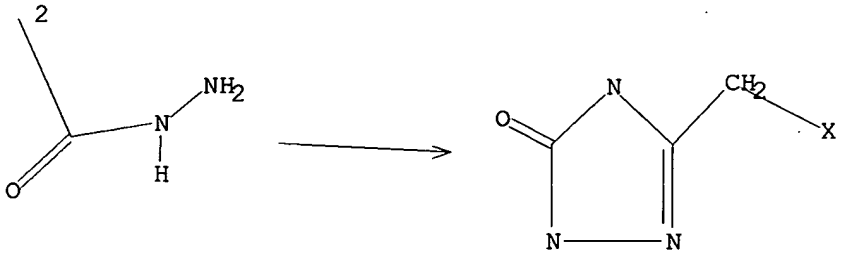


chain nodes :
1 2 3 4 5 6 14 15 16
ring nodes :
9 10 11 12 13
chain bonds :
1-2 2-3 2-4 4-5 4-6 10-15 13-14 15-16
ring bonds :
9-10 9-13 10-11 11-12 12-13
exact/norm bonds :
1-2 2-3 2-4 4-6 9-10 9-13 10-11 11-12 12-13 13-14
exact bonds :
4-5 10-15 15-16

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS
fragments assigned product role:
containing 9
fragments assigned reactant/reagent role:
containing 1

L1 STRUCTURE UPLOADED

=> D L1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> S L1 SSS SAM
SAMPLE SEARCH INITIATED 10:14:21 FILE 'CASREACT'
SCREENING COMPLETE -      0 REACTIONS TO VERIFY FROM        0 DOCUMENTS

100.0% DONE       0 VERIFIED       0 HIT RXNS                        0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:          0 TO        0
PROJECTED ANSWERS:                0 TO        0

L2            0 SEA SSS SAM L1 (     0 REACTIONS)

=> S L1 SSS FUL
FULL SEARCH INITIATED 10:14:40 FILE 'CASREACT'
SCREENING COMPLETE -     18 REACTIONS TO VERIFY FROM        6 DOCUMENTS

100.0% DONE      18 VERIFIED       6 HIT RXNS                        3 DOCS
SEARCH TIME: 00.00.01

L3            3 SEA SSS FUL L1 (     6 REACTIONS)

=> D K3 1-3 BIB HITSTR abs
'K3' IS NOT A VALID FORMAT FOR FILE 'CASREACT'
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number.  SCAN
             must be entered on the same line as DISPLAY, e.g.,
             D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for
             all single-step reactions)
STD -------- BIB, IPC, and NCL
```

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first
hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
CA reference information (SO, PY). (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction
Summary for all hit reactions and fields containing
hit terms
OCC -------- All hit fields and the number of occurrences of the
hit terms in each field. Includes total number of
HIT, PATH, SPATH reactions. Labels reactions that have
incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long
path". Displays all hit reactions, except those
whose steps are totally included within another hit
reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short
path". Displays all single step reactions which
contain a hit substance. Also displays those
multistep reactions that have a hit substance in both
the first and last steps of the reaction, except for
those hit reactions whose steps are totally included
within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):END

=> D L3 1-3 BIB HITSTR ABS
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications

ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number. SCAN must be entered on the same line as DISPLAY, e.g., D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with CA reference information (SO, PY). (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction Summary for all hit reactions and fields containing hit terms
OCC -------- All hit fields and the number of occurrences of the hit terms in each field. Includes total number of HIT, PATH, SPATH reactions. Labels reactions that have incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long path". Displays all hit reactions, except those whose steps are totally included within another hit reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):END

=> D L3 1-3 ALL

L3 ANSWER 1 OF 3 CASREACT COPYRIGHT 2006 ACS on STN
AN 140:217645 CASREACT
TI Preparation of 3-chloromethyl-1,2,4-triazolin-5-one from orthoesters and semicarbazide sulfonic acid salts.
IN Seibert, Kevin; Shultz, Clinton Scott; Tellers, David M.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 17 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
FAN.CNT 1

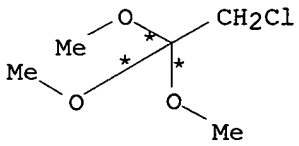
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004017898	A2	20040304	WO 2003-US25679	20030818
	WO 2004017898	A3	20040527		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2003259866	A1	20040311	AU 2003-259866	20030818
	EP 1549623	A2	20050706	EP 2003-793080	20030818
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	US 2006052355	A1	20060309	US 2005-524866	20050214
PRAI	US 2002-404843P	20020821			
	WO 2003-US25679	20030818			

OS MARPAT 140:217645
AB 3-Chloromethyl-1,2,4-triazolin-5-one was prepared by reaction of XCH2C(OR1)3 (X = halo; R1 = alkyl, aryl) with H2NCONHNH2.R2SO3H (R2 = alkyl, alkylthio, cycloalkyl, aryl) in an organic solvent (no exptl. data).
ST orthoester semicarbazide sulfonate cyclocondensation; chloromethyltriazolinone prepn
IT Esters, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(ortho acid; preparation of 3-chloromethyl-1,2,4-triazolin-5-one from orthoesters and semicarbazide sulfonic acid salts)
IT Cyclocondensation reaction
(preparation of 3-chloromethyl-1,2,4-triazolin-5-one from orthoesters and semicarbazide sulfonic acid salts)
IT 252742-72-6P, 3-Chloromethyl-1,2,4-triazolin-5-one
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 3-chloromethyl-1,2,4-triazolin-5-one from orthoesters and semicarbazide sulfonic acid salts)
IT 67-56-1, Methanol, uses 108-88-3, Toluene, uses 1634-04-4, Methyl tert-butyl ether
RL: NUU (Other use, unclassified); USES (Uses)
(preparation of 3-chloromethyl-1,2,4-triazolin-5-one from orthoesters and semicarbazide sulfonic acid salts)
IT 57-56-7D, Semicarbazide, sulfonic acid salts
RL: RCT (Reactant); RACT (Reactant or reagent)

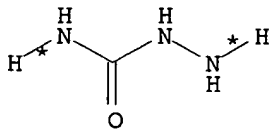
(preparation of 3-chloromethyl-1,2,4-triazolin-5-one from orthoesters and semicarbazide sulfonic acid salts)

IT 76-05-1, Trifluoroacetic acid, reactions 7647-01-0, Hydrochloric acid, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(preparation of 3-chloromethyl-1,2,4-triazolin-5-one from orthoesters and semicarbazide sulfonic acid salts)

RX(1) OF 1 A + **B** ===> **C**

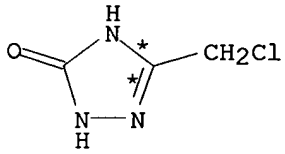


A



B
sulfonic acid salts

(1) ⟶



C

RX(1) RCT A 74974-54-2, B **57-56-7D**

STAGE(1)
CON SUBSTAGE(1) room temperature -> 42 deg C
SUBSTAGE(2) 16 hours

STAGE(2)
RGT D 7647-14-5 NaCl
SOL 7732-18-5 Water
CON 25 - 35 deg C

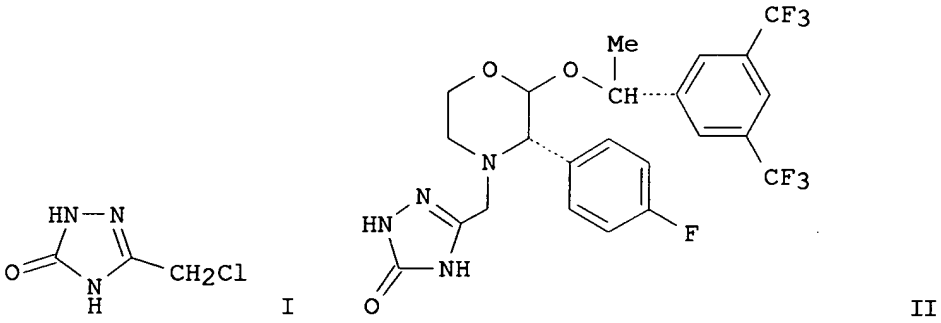
PRO C **252742-72-6**

L3 ANSWER 2 OF 3 CASREACT COPYRIGHT 2006 ACS on STN
AN 136:37612 CASREACT
TI Process for the preparation of 1,2,4-triazolin-5-one derivatives
IN Cowden, Cameron John
PA Merck Sharp & Dohme Limited, UK
SO PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D249-12

ICS C07D413-06
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001096315	A1	20011220	WO 2001-GB2617	20010613
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2411366	AA	20011220	CA 2001-2411366	20010613
	AU 2001074226	A5	20011224	AU 2001-74226	20010613
	AU 781139	B2	20050505		
	EP 1294703	A1	20030326	EP 2001-940722	20010613
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2004503543	T2	20040205	JP 2002-510458	20010613
	US 2003187274	A1	20031002	US 2003-311389	20030205
	US 6673939	B2	20040106		
PRAI	GB 2000-14876	20000616			
	WO 2001-GB2617	20010613			

OS MARPAT 136:37612
GI

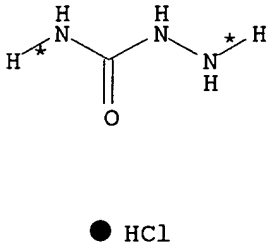


AB Triazolinones such as I were prepared and reacted with morpholine derivs. to give products such as II, which are useful therapeutic agents, e.g., substance P receptor antagonists. Thus, I was prepared in 98% yield from semicarbazide hydrochloride and ClCH2C(OMe)3, and reaction of I with (2R)-[(1R)-[3,5-bis(trifluoromethyl)phenyl]ethoxy]-(3S)-(4-fluorophenyl)morpholine p-toluenesulfonic acid salt gave II in 99.7% yield.

ST triazolinone morpholinomethyl prepn
IT 930-33-6P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of 1,2,4-triazolin-5-ones)
IT 170729-80-3P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,2,4-triazolin-5-ones)

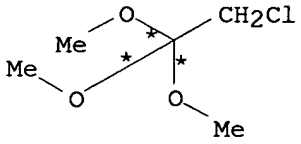
IT 149-73-5, Trimethyl orthoformate 563-41-7, Semicarbazide hydrochloride
74974-54-2 200000-59-5 252742-71-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 1,2,4-triazolin-5-ones)
IT 252742-72-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1,2,4-triazolin-5-ones)
RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Cowden, C; TETRAHEDRON LETTERS 2000, 41, P8661
(2) Kamata, K; HETEROCYCLES 1999, V51(2), P373 CAPLUS
(3) Lonza Ag; WO 9918089 A 1999 CAPLUS
(4) Merck Sharp & Dohme; WO 9965900 A 1999 CAPLUS

RX(1) OF 4 **A** + B ===> **C**...



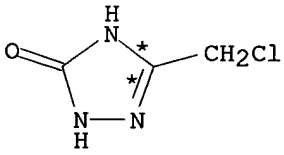
● HCl

A



B

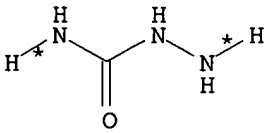
(1) →



C
YIELD 98%

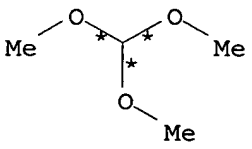
RX(1) RCT A **563-41-7**, B 74974-54-2
PRO C **252742-72-6**
SOL 67-56-1 MeOH

RX(2) OF 4 A + E ===> F



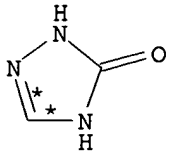
● HCl

A



E

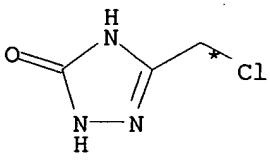
(2) ⟶



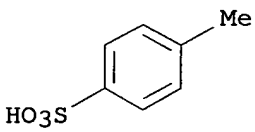
F
YIELD 100%

RX(2) RCT A 563-41-7, E 149-73-5
PRO F 930-33-6
SOL 67-56-1 MeOH

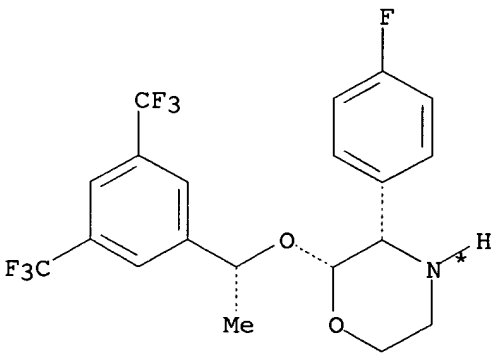
RX(3) OF 4 ...C + G ===> H



C

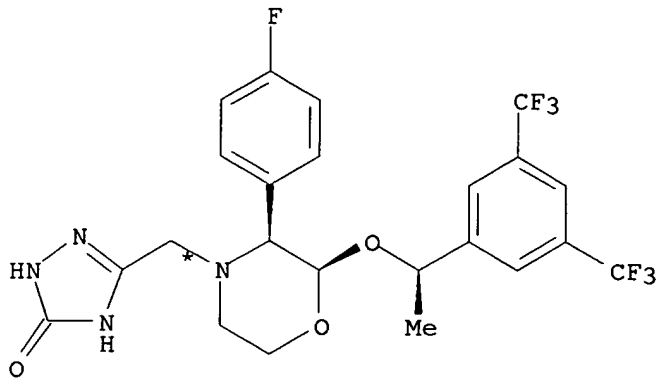


G: CM 1



G: CM 2

(3) ⟶



H
YIELD 99%

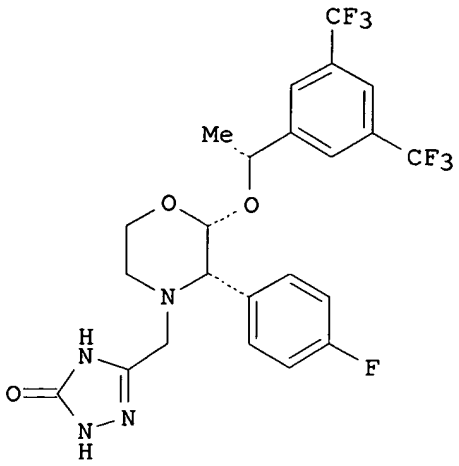
RX(3) RCT C 252742-72-6, G 200000-59-5

STAGE(1)
RGT I 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF

STAGE(2)
SOL 7732-18-5 Water

PRO H 170729-80-3
NTE alternative prepn. gave lower yields

L3 ANSWER 3 OF 3 CASREACT COPYRIGHT 2006 ACS on STN
AN 134:115901 CASREACT
TI A new synthesis of 1,2,4-triazolin-5-ones: application to the convergent synthesis of an NK1 antagonist
AU Cowden, Cameron J.; Wilson, Robert D.; Bishop, Brian C.; Cottrell, Ian F.; Davies, Antony J.; Dolling, Ulf-H.
CS Department of Process Research, Merck Sharp and Dohme Research Laboratories, Hoddesdon, EN11 9BU, UK
SO Tetrahedron Letters (2000), 41(44), 8661-8664
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
GI



II

AB 3-Chloromethyl-1,2,4-triazolin-5-one (I) has been synthesized in a single step via the novel condensation of semicarbazide hydrochloride with ClCH2C(OMe)3. Alkylation of the secondary amine fragment with I proceeds in 99% yield to afford the target NK1 antagonist II.

ST chloromethyltriazolinone prepn alkylation morpholine; triazolinone chloromethyl prepn alkylation morpholine; morpholinylmethyltriazolinone NK1 antagonist prepn

IT 79-07-2P, Acetamide, 2-chloro-
RL: AMX (Analytical matrix); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)
(preparation of 3-chloromethyl-1,2,4-triazolin-5-one and its application to the convergent synthesis of an NK1 antagonist)

IT 107-14-2, Chloroacetonitrile 563-41-7, Semicarbazide hydrochloride 1634-04-4, tert-Butyl methyl ether 19810-31-2, Benzyloxyacetyl chloride 74974-54-2, Trimethyl orthochloroacetate 321125-96-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 3-chloromethyl-1,2,4-triazolin-5-one and its application to the convergent synthesis of an NK1 antagonist)

IT 24021-90-7P 70737-12-1P, Methyl chloroacetimidate hydrochloride 252742-72-6P 252742-73-7P 321125-97-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3-chloromethyl-1,2,4-triazolin-5-one and its application to the convergent synthesis of an NK1 antagonist)

IT 321125-94-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 3-chloromethyl-1,2,4-triazolin-5-one and its application to the convergent synthesis of an NK1 antagonist)

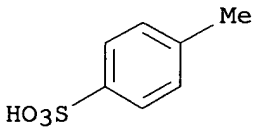
RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

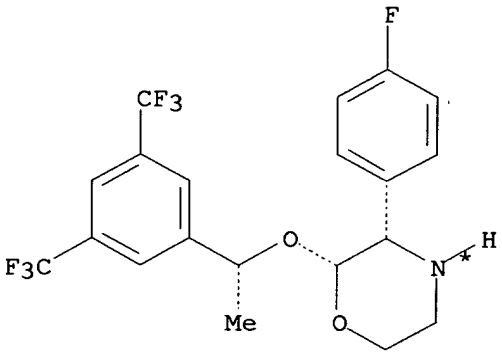
(1) Adembri, G; J Chem Soc Perkin Trans 1 1981, P1703 CAPLUS
(2) Hale, J; J Med Chem 1998, V41, P4607 CAPLUS
(3) Kamata, K; Heterocycles 1999, V51, P573
(4) McElvain, S; J Am Chem Soc 1942, V64, P1825 CAPLUS
(5) Milcent, R; J Heterocycl Chem 1986, V23, P881 CAPLUS
(6) Moos, W; J Org Chem 1981, V46, P5064 CAPLUS
(7) Mylari, B; J Synth Commun 1989, V19, P2921 CAPLUS
(8) Regoli, D; Pharmacol Rev 1994, V46, P551 CAPLUS
(9) Rigo, B; Synth Commun 1988, V18, P167 CAPLUS
(10) Scott, F; J Chem Soc Perkin Trans 1 1972, P1918 CAPLUS
(11) Shvaika, O; Dokl Akad Nauk SSSR 1969, V186, P1102 CAPLUS

(12) Un, R; Chim Acta Turc 1975, V3, P113 CAPLUS

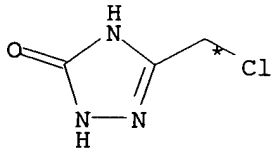
RX(1) OF 24 ...A + B ===> C



A: CM 1

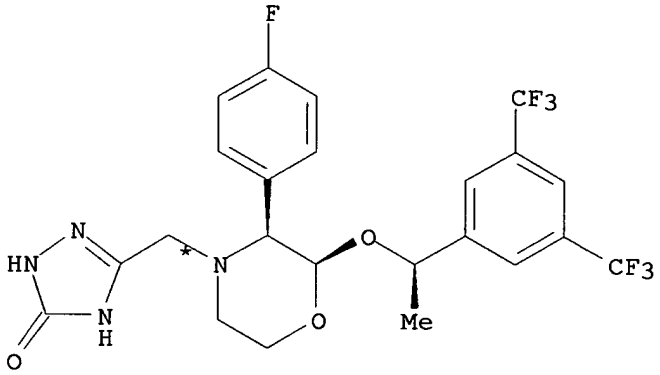


A: CM 2



B

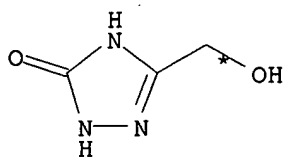
(1)



C
YIELD 99%

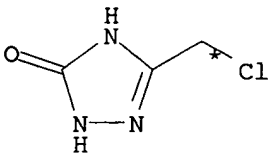
RX(1) RCT A 321125-96-6, B 252742-72-6
RGT D 584-08-7 K2CO3
PRO C 321125-94-4
SOL 68-12-2 DMF, 7732-18-5 Water
NTE alternate base gave similar yields

RX(2) OF 24 ...G ===> B...



G

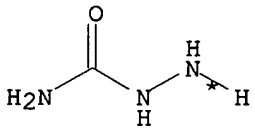
(2)



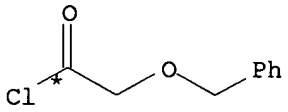
B
YIELD 87%

RX(2) RCT G 24021-90-7
RGT H 7719-09-7 SOCl2
PRO B 252742-72-6
SOL 75-05-8 MeCN

RX(3) OF 24 J + K ===> L...

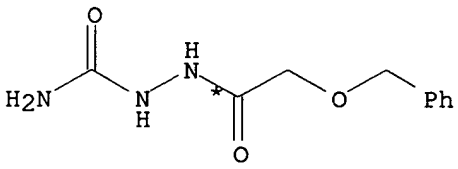


● HCl



J K

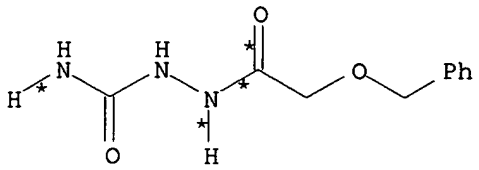
(3)



L

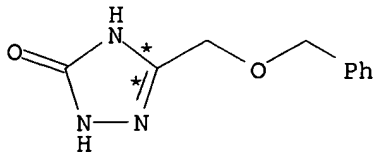
RX(3) RCT J 563-41-7, K 19810-31-2
RGT M 1310-73-2 NaOH
PRO L 321125-97-7
SOL 109-99-9 THF, 7732-18-5 Water

RX(4) OF 24 ...L ===> O...



L

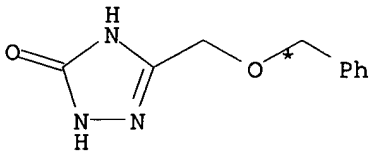
(4)



O
YIELD 60%

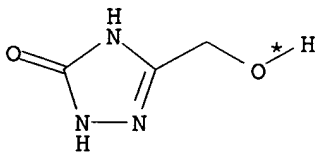
RX(4) RCT L 321125-97-7
RGT M 1310-73-2 NaOH
PRO O 252742-73-7
SOL 7732-18-5 Water

RX(5) OF 24 ...O ===> G...



O

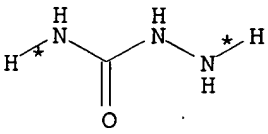
(5)



G
YIELD 98%

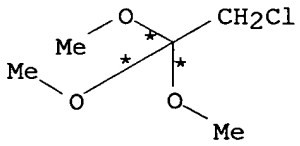
RX(5) RCT O 252742-73-7
RGT P 540-69-2 Ammonium formate
PRO G 24021-90-7
CAT 7440-05-3 Pd
SOL 7732-18-5 Water, 67-56-1 MeOH

RX(6) OF 24 ...**J** + S ===> **B**...



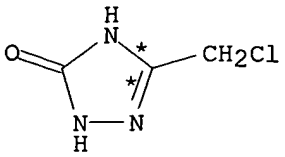
● HCl

J



S

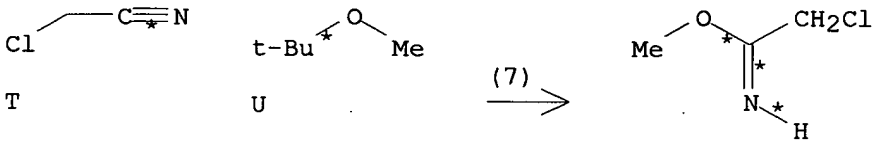
(6)



B
YIELD 98%

RX(6) RCT J **563-41-7,** S 74974-54-2
PRO B **252742-72-6**
SOL 67-56-1 MeOH

RX(7) OF 24 T + U ===> V...



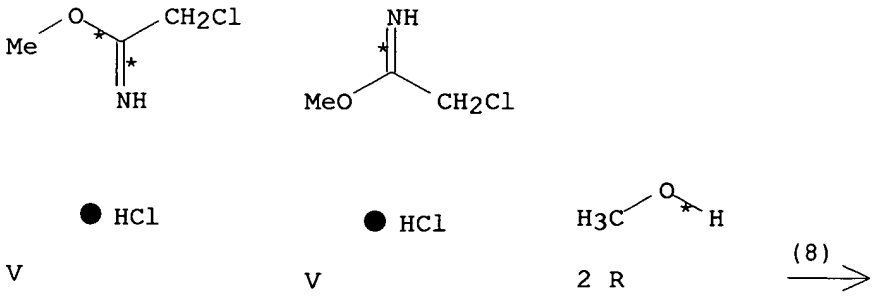
T U

● HCl

V
YIELD 95%

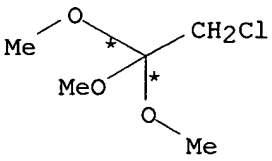
RX(7) RCT T 107-14-2, U 1634-04-4
RGT W 7647-01-0 HCl
PRO V 70737-12-1
SOL 7732-18-5 Water

RX(8) OF 24 ...2 V + 2 R ===> S + X...

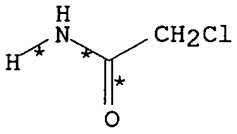


● HCl ● HCl

V V 2 R



S



X

RX(8) RCT V 70737-12-1, R 67-56-1
PRO S 74974-54-2, X 79-07-2
SOL 67-56-1 MeOH
NTE combined yield of 65%

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	137.67	137.88

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.13	-2.13

STN INTERNATIONAL LOGOFF AT 10:17:49 ON 05 MAY 2006